Note: Today's lecture was created **without** the use of AI

Florin Bobaru, Sept. 4th, 2025

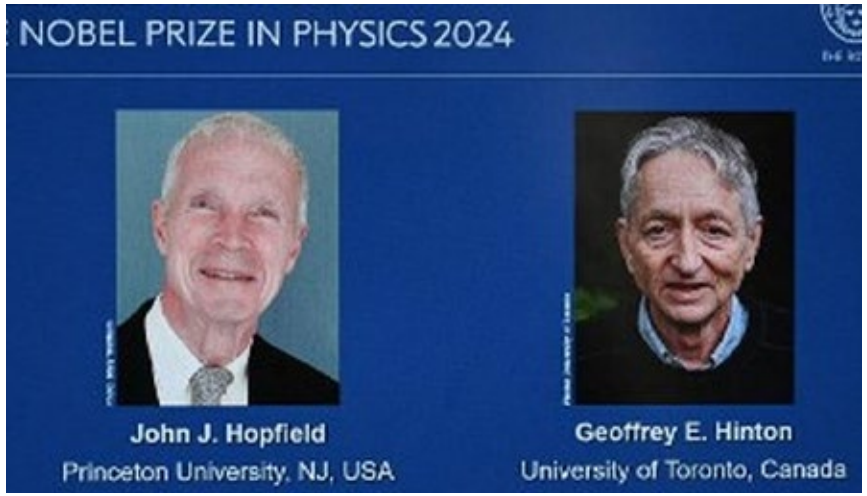
AI and Artificial Neural Networks

The Good, the Bad, and the Ugly

Prof. Florin Bobaru

Mechanical and Materials Engineering
University of Nebraska-Lincoln
Sept 4, 2025

The Why



- John Hopfield and Geoffrey Hinton: 2024 Nobel Prize in physics ***"for foundational discoveries and inventions that enable machine learning with artificial neural networks."***
- "These artificial neural networks have been **used to advance research across physics** topics as diverse as particle physics, material science, and astrophysics. They have also become part of our daily lives, for instance, in facial recognition and language translation." (Ellen Moons, chair of the Nobel Committee for Physics)
- "However, while machine learning has enormous benefits, its rapid development has also raised concerns about our future. Collectively, humans carry the responsibility for **using this new technology in a safe and ethical way** for the greatest benefit of humankind (Ellen Moons, chair of the Nobel Committee for Physics)

The Good

- Explosion once applications in computer vision and natural language processing were shown (circa 2012, 2017).
- Medicine: medical image identification (e.g., detection of cancer, ECG interpretation to detect heart conditions, etc.)
- Materials Science:
  - Atomic Cluster Expansion (ACE): fast and accurate ML force fields
  - Data acquisition, experiments
- Mechanical Engineering:
  - Robotics, autonomous vehicles/drones
  - Mechanical deformation and motion, weather forecasting, PINNs
  - Coding
- Numerical Linear Algebra (https://doi.org/10.1137/23M1609786)

The Bad (e.g. cybercrime)

- Cybercrime increased 1200% since 2023

- “A hacker exploited Anthropic chatbot to conduct the most comprehensive and lucrative AI cybercriminal operation known to date, using it to find targets, write ransom notes…. The hacker used the chatbot to automate almost an entire cybercrime spree.” (NBC News, 08/27/2025)
  - identify companies vulnerable to attack
  - created malicious software to steal sensitive information from the companies.
  - organized the hacked files and analyzed them to both help determine what was sensitive and could be used to extort the victim companies.
  - analyzed the companies’ hacked financial documents to help determine a realistic amount of bitcoin to demand in exchange for the hacker’s promise not to publish that material.
  - wrote suggested extortion emails.

The Ugly

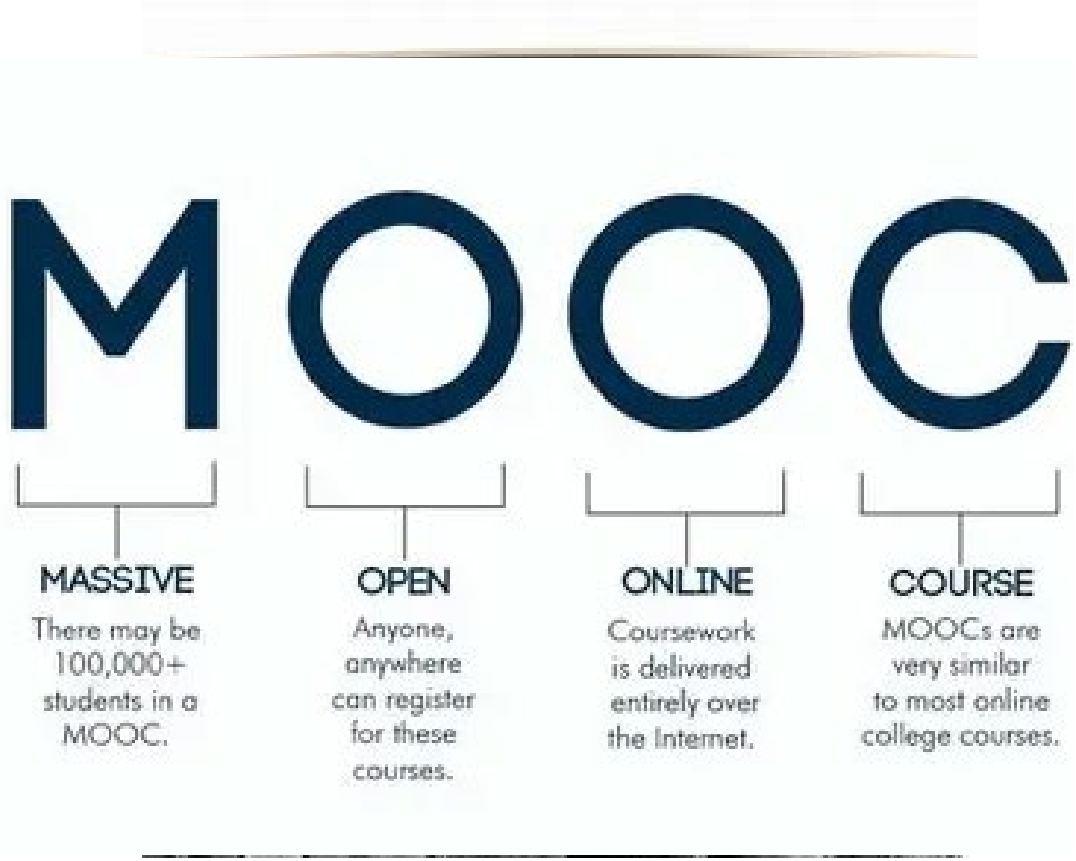
- ChatGPT May Be Eroding Critical Thinking Skills (https://time.com/7295195/ai-chatgpt-google-learning-school/ https://arxiv.org/pdf/2506.08872v1)

- Role of generative AI in schools: *"Colleges should go 'medieval' on students to beat AI cheating"* (NY Time, 08/26/2025, Clay Shirky, NYU vice-provost for AI and technology in education) https://www.nytimes.com/2025/08/26/opinion/culture/ai-chatgpt-college-cheating-medieval.html

- Watch for a round-table discussion later in the semester on *"Using AI in MME responsibly"*

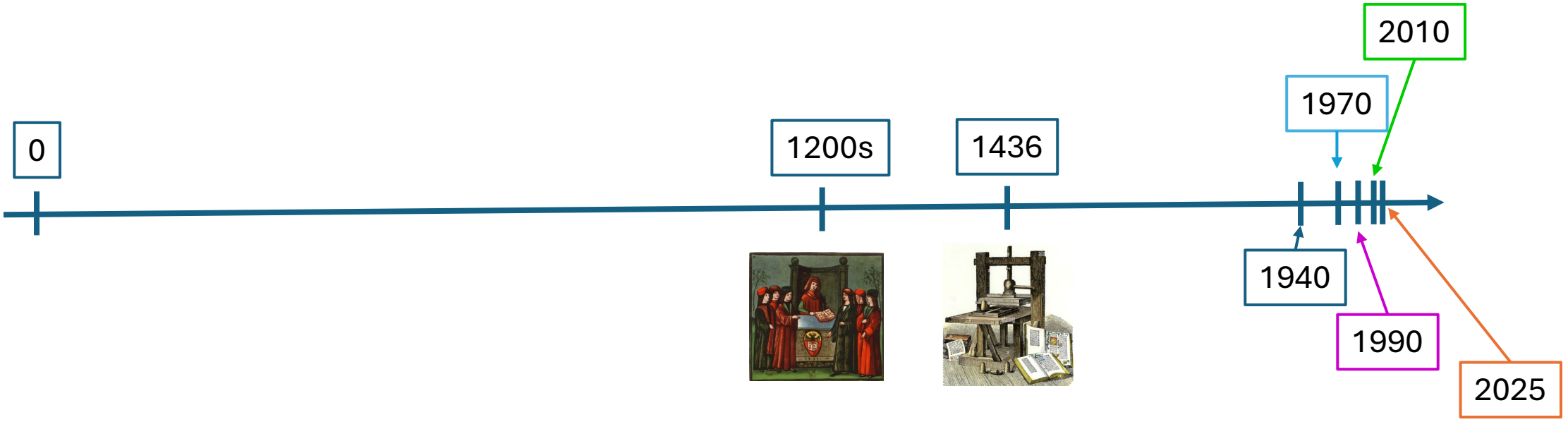
Does college still have a purpose?

- Circa 1440s: “College is doomed because students can now get an education from **the printing press**
- Circa 1940s and 1970s: “College is doomed because students can now get an education from **Radio or TV**”
- Circa 2010s:“College is doomed because students can now get an education from **free online courses**”
  - Advantages of Online Learning: flexibility/comfort, self-paced, chat-rooms, discussion forums, cost.
  - Disadvantages of Online Learning: lack of personal interaction, difficult to focus, ask questions but cannot get immediate feedback from teachers and classmates, no chance to build interpersonal relationships with others.



Does college still have a purpose?

- Circa 2025: :“College is doomed because students can now get an education from **generative AI tutors**”



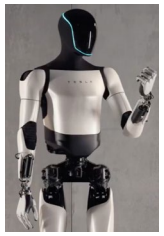
Why this is not likely to happen

- “…college is not in the information transfer business; we are in the **identity formation** business” (Clay Shirky)

- “In a time when many worry about AI replacing jobs, teaching may be one of the most resilient professions because it thrives on what no machine can replicate: **trust, encouragement, and connection**.” (Salman Khan, Newsweek, Sept. 2025)

Likely ways in which AI will impact research in MME

- Automate tedious tasks (e.g. tools to research/summarize existing literature faster, insert/cite references faster, etc.) to allow more time for creativity
- Make difficult things simple (e.g. writing code). Need to verify it!
- Offer new research ideas/topics:
  - Autonomous robotics (vision, motion)
  - Equation-free/data-driven models for fluid flow, heat transfer, deformation and damage
  - Design of materials (e.g. defect-tolerant metamaterials)
  - The Energy question: MME can help!



What's in the black box?
Introduction to Deep Neural Networks

Goals

- Basic understanding of DNNs
- Strong foundation for future explorations:
  - Physics-Informed Neural Networks (**PINNs**)
  - Convolutional Neural Networks (CNNs)
  - Generative Adversarial Networks (GANs)
  - Graph Neural Networks (GNNs)
  - Transformers, etc.

What will you learn in these lectures?

- What is a Deep Neural Network (DNN)?
- How are NNs trained and used?
- What is the Stochastic Gradient Method (SGD) or variants (e.g. Adam)?
- “Backpropagation” or Automatic Differentiation (AD)

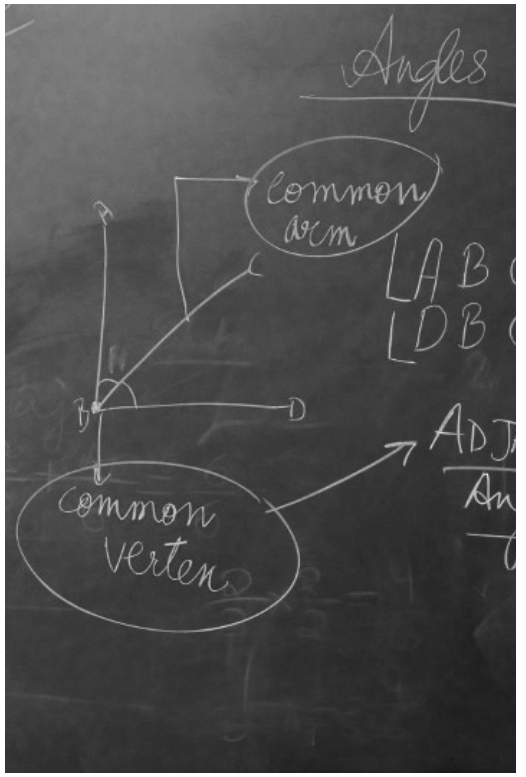
- Approach ANNs from a **data fitting** (aka “**surrogate models**”) POV
- Start with “regular” curve fitting

Background needed

- Linear Algebra
- Calculus, partial derivatives
- Basic scientific computing

Teaching style

- “Medieval”
- Taking notes helps retention
- Practical exercises



Steps beyond

- MECH 888 (Nonlinear Optimization in Engineering), Spring 2026
- Courses in ECE, SoC, Math

References

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